

## A Generic Methodology for Superstructure Optimization of Different Processing Networks - DTU Orbit (09/11/2017)

### A Generic Methodology for Superstructure Optimization of Different Processing Networks

A large focus is placed on sustainability and sustainable practices as a result of the arising environmental issues. As an element of this, sustainable process synthesis and design becomes important. A generic, systematic methodology is proposed for solving the problem of optimal design of sustainable processing networks containing three stages: (i) synthesis stage, (ii) design stage, and (iii) innovation stage. In this work, a focus is placed on the first stage, the synthesis stage. Process synthesis becomes necessary in determining the appropriate processing routes to produce a selection of products from a set or feedstock. The problem to be solved here is the following: for a given set of raw materials, products and a network of processing routes, determine the optimal processing route from a sustainability point of view. Three different processing networks arising from chemical processes, biorefineries, and carbon dioxide utilization are considered. In the synthesis stage, the processing alternatives are represented in a superstructure and the associated data is collected and stored in a database. Once a specific process synthesis problem is formulated, the existing superstructure is retrieved and reduced in order to include only the relevant alternatives. New alternatives can easily be added and stored in the database. The superstructure of alternatives in the network is then represented using a generic data-independent process model, which yields a mixed integer linear or nonlinear programming problem. The proposed methodology involves the use of additional methods and tools, such as a database and an external software for solving the network optimization problem. The database has been created using an ontology-based knowledge representation consisting in various layers of data and interconnections between them. Using a common database structure for any process synthesis problem allows for easy data collection, storage and retrieval, as well as giving the possibility of solving combined problems that have been previously solved independently. The step-by-step methodology has been implemented in a software interface that guides the user through the problem formulation and solution steps and integrates the various methods and tools for efficient flow of information between them. By using this interface, the user can retrieve and/or modify existing networks and alternatives from the database, as well as add new alternatives and connections between them. With the generated superstructure of alternatives and the corresponding data, an input file for GAMS is automatically created. This input file contains values of all the parameters of the generic process model. Then, the problem is solved in GAMS and the interface shows the results and allows for the selection of alternatives. The output from the synthesis stage (the first stage) is the optimal processing route for the defined problem and scenario, which can be transferred to a rigorous process simulator for the second stage (design stage). Here, the selected route needs to be further designed, simulated and analyzed. Then, more sustainable innovative designs can be developed in the third stage based on the output design from the second stage. This generic methodology and software interface can be applied to an array of problems within synthesis of processing networks. This is illustrated through case studies from two applications: the synthesis of biorefinery networks and the synthesis of sustainable carbon dioxide utilization processes.

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